

**Table S3 Comparison of simulated versus observed dapagliflozin concentration values.**

Dataset	Dose	Points outside deviation range [0.5, 2] (number)	Points outside deviation range $[0.7, \frac{1}{0.7}]$ (number)
i)	1 mg/kg	1	3
ii)	6.6 mg/kg	1	3
iii)	6 mg/kg	3	7
iv)	80 µg	0	2
v)	50 mg	1	1
vi)	2.5 mg	0	2
-	5 mg	1	3
-	10 mg	0	0
-	20 mg	0	2
-	50 mg	0	0
-	100 mg	0	0
-	250 mg	0	1
-	500 mg	0	2
vii)	2.5 mg	0	5
-	10 mg	0	1
-	20 mg	0	2
-	50 mg	0	1
-	100 mg	0	1
viii)	10 mg	0	1
Total of 369 points		7 (1.9%)	37 (10%)

A total of 369 mean concentration values observed in 19 experiments are compared with simulated values. For each dataset, the numbers of points outside of the defined deviation ranges  $[0.5, 2]$  and  $[0.7, \frac{1}{0.7}]$  are reported. Datasets are numbered as in Supplementary Table S3.